Localization-Delocalization Transition in the Random Dimer Model

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The random-dimer model is probably the most popular model for a one-dimensional disordered system where correlations are responsible for delocalization of the wave functions. This is the primary model used to justify the insulator-metal transition in conducting polymers and in DNA. However, for such systems, the localization-delocalization regimes have only been observed by deeply modifying the system itself, including the correlation function of the disordered potential. In this article, we propose to use an ultracold atomic mixture to cross the transition simply by externally tuning the interspecies interactions, and without modifying the impurity correlations.

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In a one-dimensional disordered system, Anderson localization is known to occur at any energy when the disorder is δ correlated [1, 2]. Nevertheless, if one introduces particular short-range correlations, delocalization of a significant subset of the eigenstates can appear. This happens in the random-dimer model (RDM) [3], in which the sites of a lattice are assigned energies ϵ_a or ϵ_b at random, with the additional constraint that sites of energy ϵ_b always appear in pairs, or dimers. The same occurs in its dual counterpart (DRDM) [3], in which lattice sites with energy ϵ_h never appear as neighbors. In these models, extended states arise from resonant modes of the (dual)dimers which present vanishing backscattering at energy $E_{\rm res}$. In the thermodynamic limit, the ratio $\sqrt{N/N}$ between the number of delocalized states and the total number of states vanishes, and there is no mobility edge separating extended and localized energy eigenstates. Nevertheless in finite size systems, thus in real systems, a localization-delocalization transition can be induced by driving $E_{\rm res}$ inside the spectrum.

This model was proposed to be the possible mechanism which leads to the insulator-metal transition in a wide class of conducting polymers such as polyaniline and heavily doped polyacetylene (see, for instance, [4]) and in some biopolymers such as DNA [5, 6]. The evidence of delocalized electronic states was experimentally demonstrated in a random-dimer GaAs-AlGaAs superlattice [7], while for photons, a RDM dielectric system was used [8]. Recently, a RDM setup has been proposed to demonstrate the delocalization of acoustic waves [9]. For polymers, semiconductor lattices, photonic crystals and elastic chains, the dimer resonant energies cannot be modified without changing the sample itself. Thus the localization-delocalization transition for a (D)RDM chain as a function of the relative position of the resonant modes with respect to the band modes cannot easily be studied using these physical systems.

In this article, we propose an experimental procedure to realize a DRDM experiment with a one-dimensional (1D) two-component ultracold atomic mixture in an optical lattice, and we demonstrate that the localization-delocalization transition can be explored by tuning the interparticle interactions.

To introduce disorder, a component (B_d) has to be classically trapped in the minima of the potential [10-12]. For this purpose, one can choose a spin-polarized Fermi component or a strongly repulsive hardcore Bose gas. The other component (B_f) must be able to tunnel through the potential maxima. A single impurity B_d trapped in a lattice site causes an energy shift of the effective potential seen by the second species B_f with respect to the case where the impurity is absent. In the following we will focus on a boson-boson mixture, taking recent experiments on the ⁴¹K-⁸⁷Rb mixture at LENS as a guide [13]. This mixture has tunable interspecies interactions for both 87 Rb and 41 K in the $|F=1,m_f=$ 1) state [14]. The ⁴¹K condensed component plays the role of the "tunnelling bosons" B_f and the heavier $^{87}\mathrm{Rb}$ atoms are the defects B_d .

To study the effect of correlated impurities B_d on matter-wave transport, we use the 1D effective tight-binding (TB) Hamiltonian for bosons B_f ,

$$H_{B_f} = \sum_{i=1}^{n_s} E_i |i\rangle\langle i| + \sum_{i=1}^{n_s - 1} t_i (|i\rangle\langle i + 1| + |i + 1\rangle\langle i|)$$
 (1)

where n_s is the number of sites, $E_i \in \{\epsilon_a, \epsilon_b\}$, and ϵ_b 's never appear as neighbors. The hopping term t_i can take the values t_{aa} between two sites with energy ϵ_a or t_{ab} between two sites with different energies. The constraint on sites with energy ϵ_b fixes the hopping energies t_{ab} to be distributed as "dual dimers" of the form $\epsilon_a \stackrel{t_{ab}}{\frown} \epsilon_b \stackrel{t_{ab}}{\frown} \epsilon_a$. To realize such an experiment, one needs to assure that there can be either zero or one impurity B_d in each lattice site and that they never appear in succession. The procedure we propose is schematized in Fig. 1. (i) First, N_{B_d} atoms of species B_d are trapped in a lattice with a step 3d, with the condition that no site must be doubly occupied, as in the Tonks gas experiment described in [15]. Such a lattice can be realized using beams of

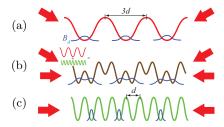


FIG. 1: (Color online) Experimental scheme to generate the correlated disorder. (a) Impurities are trapped in a lattice of step 3d. (b) A second lattice of step d is switched on, and the first one turned off. In the final configuration (c), the impurities follow a DRDM distribution.

wavelength $\lambda = 2d$, tilted by an angle $\alpha = a\cos(1/3)$ [see Fig. 1(a)]. For the case $\lambda=800\,\mathrm{nm}$ and a lattice potential depth $U_{B_d}^{0,in}\simeq30E_{B_d},\,E_{B_d}=4\pi^2\hbar^2/(2m_{B_d}\lambda^2)$ being the recoil energy for a boson of mass m_{B_d} , and for an axial confinement of $2\pi \times 60$ Hz [15], double occupancy can be avoided if $N_{B_d} \leq 20$ [16]. The number of impurities can be increased by increasing the lattice potential depth or by relaxing the axial confinement. (ii) Then impurities are forbidden to occupy neighbor sites by adiabatically ramping up the power in a second superimposed lattice of step d, and switching off the first one [17]. The potential depth $U_{B_d}^0$ of the final lattice $U_{B_d,B_f}(z) = U_{B_d,B_f}^0 \sin^2(\pi z/d)$ must be large compared to E_{B_d} to neglect the impurity mobility during the experiment course (0.5 to 1 s [18, 19]). This condition can be fulfilled at $U_{B_d}^0 = 18E_{B_d}$ in the presence of attractive interactions with the species B_f . Differently, the depth $U_{B_f}^0$ for the species B_f must be $\gtrsim 2 E_{B_f}$, the recoil energy for a B_f boson, to guarantee the validity of the TB description.

The effective Hamiltonian (1) is obtained by a 1D reduction of the system Hamiltonian by introducing the transverse widths $\sigma_{\perp B_f,B_d}$ of the condensate and of the impurities wave functions in a cylindrical trap [20]. Using a TB scheme we introduce the Wannier function $\phi_i(z)$ approximated by the Gaussian function $\phi_i(z) = [\phi_i(0)/(\pi^{1/4}\sigma_{zB_f}^{1/2})] \exp[-(z-z_i)^2/(2\sigma_{zB_f}^2)]$, where $|\phi_i(0)|^2$ is the number of bosons B_f in the lattice well i. Similarly, the density of impurities is $n_{B_d} \propto \sum_{i'} \exp[-(z-z_{i'})^2/\sigma_{z,B_d}^2]$. The determination of the widths $\sigma_{\perp B_f,B_d}$ and σ_{zB_f,B_d} is carried out variationally [10, 20].

We can now evaluate the parameters entering the effective Hamiltonian (1). The site energies are given by

$$E_{i} = \int dz \, \tilde{\phi}_{i}(z) \left[-\frac{\hbar^{2} \nabla^{2}}{2m_{B_{f}}} + U_{B_{f}}(z) + \frac{1}{2} g |\phi_{i}(z)|^{2} + g' n_{B_{d}}(z) + C_{B_{f}} \right] \tilde{\phi}_{i}(z)$$
(2)

where m_{B_f} is the mass of the boson B_f , C_{B_f}

 $\hbar^2/(2m_{B_f}\sigma_{\perp\,B_f}^2) + \frac{1}{2}m_{B_f}\omega_{\perp\,B_f}^2\sigma_{\perp\,B_f}^2$, and $\omega_{\perp\,B_f}$ is the radial frequency of the harmonic trapping potential. $\tilde{\phi}_i(z)$ are modified Gaussian functions, obtained by imposing the condition $\int \tilde{\phi}_i(z) \tilde{\phi}_j(z) = \delta_{ij}$ [21]. The parameters g and g' are the strengths of the 1D $B_f B_f$ and $B_f B_d$ interactions, which are given by $g = (4\pi\hbar^2 a)/(2\pi m_{B_f}\sigma_{\perp\,B_f}^2)$ and $g' = (2\pi\hbar^2 a')/[\pi m_r(\sigma_{\perp\,B_f}^2 + \sigma_{\perp\,B_d}^2)]$, with a,a' the $B_f B_f$ and the $B_f B_d$ scattering lengths and m_r the $B_f B_d$ reduced mass. The hopping energies t_i are given by

$$t_i = \int dz \,\tilde{\phi}_i(z) \left[-\frac{\hbar^2 \nabla^2}{2m_{B_f}} + U_{B_f}(z) \right] \tilde{\phi}_{i+1}(z). \tag{3}$$

This completes the determination of the effective 1D Hamiltonian for bosons B_f .

Delocalization occurs for energy values near to the resonance energy of a single dual dimer embedded in a perfect lattice of site energies ϵ_a and hopping energies t_{aa} . For such Hamiltonian H, the wave function at energy E is $|\varphi\rangle = |k\rangle + G^0 T |k\rangle$, where $|k\rangle$ is the wave function of the unperturbed periodic Hamiltonian $H_0 = \sum_{n=-\infty}^{\infty} \epsilon_a |n\rangle\langle n| + t_{aa}(|n\rangle\langle n+1| + \text{c.c.}), G^0$ the unperturbed Green's function $G^0(E) = (E - H_0)^{-1}$, and T the matrix $T(E) = H_{\rm I}(1 - G^0 H_{\rm I})^{-1}$, where $H_{\rm I}$ is a remainder defined as $H_{\rm I} = H - H_0 = (\epsilon_b - \epsilon_a)|0\rangle\langle 0| + (t_{ab} - t_{ab})|0\rangle\langle 0|$ t_{aa})($|-1\rangle\langle 0|+|0\rangle\langle 1|+c.c.$). Here and below the complex energy E is considered in the limit of vanishing positive imaginary part. Using the renormalization scheme outlined in [22] the scattering T matrix in the subspace $\{|-1\rangle, |1\rangle\}$ can be written as $T = \tilde{H}_{\rm I}(\mathbf{1} - G^0\tilde{H}_{\rm I})^{-1}, \tilde{H}_{\rm I}$ being the renormalized remainder Hamiltonian. We find $\tilde{H}_{\rm I} = \alpha \left(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix} \right)$ with $\alpha = t_{ab}^2/(E - \epsilon_b) - t_{aa}^2/(E - \epsilon_a)$. Thus, the scattering matrix on the subspace $\{|-1\rangle, |1\rangle\}$ is identically null if $\alpha = 0$. This occurs at the resonance energy

$$E_{\rm res} = \frac{\epsilon_a t_{ab}^2 - \epsilon_b t_{aa}^2}{t_{ab}^2 - t_{aa}^2}.$$
 (4)

Eigenstates are delocalized if $E_{\rm res}$ is inside the lowestenergy band $E(k) = \epsilon_a + 2t_{aa}\cos(kd)$, namely if $|\Delta\epsilon|$ $2|t^2-1|$, with $\Delta\epsilon=(\epsilon_b-\epsilon_a)/t_{aa}$ and $t=t_{ab}/t_{aa}$, as found by Dunlap and collaborators [3]. The corresponding phase diagram in the $(t, \Delta \epsilon)$ plane is shown in Fig. 2. The central lobe corresponds to the case where the presence of an impurity is disadvantageous to the hopping of a boson B_f . In this region delocalization occurs only for values of ϵ_b near the center of the band. The left side of the diagram corresponds to an increase of the hopping probability due to the impurities. In this region the energy value ϵ_b can be in the gap; thus, the disorder strength can be very large, but delocalization is established just by the value of E_{res} . If E_{res} is not an energy value of the spectrum, for a sufficiently long lattice, all states are localized.

For the evaluation of the site and hopping energies, we consider a system of $N_{B_f}=1.3\times 10^4$ ⁴¹K atoms distributed in 200 wells, 10% of which are occupied by

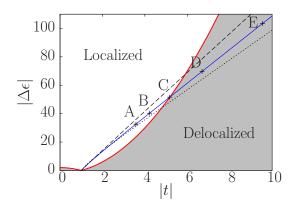


FIG. 2: (Color online) Phase diagram of the DRDM in the plane $(t, \Delta \epsilon)$, with $t = t_{ab}/t_{aa}$ and $\Delta \epsilon = (\epsilon_b - \epsilon_a)/t_{aa}$ and calculated trajectories for different number of atoms N_{B_f} obtained by varying the interspecies scattering length a'. Dashed line, $N_{B_f} = 1.6 \times 10^4$, $a' \in [0, -87 \, a_0]$; continuous line, $N_{B_f} = 1.3 \times 10^4$, $a' \in [0, -380 \, a_0]$; dotted line, $N_{B_f} = 1.0 \times 10^4$, $a' \in [0, -570 \, a_0]$. With 1.3×10^4 atoms, the localization-delocalization transition for the $B_f B_d$ mixture occurs for $a' = -346 \, a_0$ (point C). Other points correspond to a' = -316 (A), -331 (B), -361 (D), and $-376 \, a_0$ (E), respectively, a_0 being the Bohr radius.

a $^{87}\mathrm{Rb}$ atom. We choose the depth $U^0_{B_f}$ equal to 2.5 E_{B_f} and the optical lattice wavelength $\lambda=800$ nm (red detuned for both species). For linearly polarized beams, this fixes the potential depth $U^0_{B_d}$ for the defects to 18 E_{B_d} , and impurity tunneling time of the order of 1 s for points A to E in Fig. 2. The effect of the interactions is enhanced by a tight radial confinement $\omega_{\perp\,B_f}/2\pi=60$ kHz. For such a system the phase diagram can be explored just by varying the B_fB_d scattering length a' (lines in Fig. 2). In the experiments this can be done by exploiting interspecies Feshbach resonances [14]. The point (1,0) corresponds to a'=0: species B_f do not interact with impurities; thus, neither site nor hopping energies are modified by the presence of B_d and the lattice is not disordered. Higher points of the curve correspond to greater and greater attractive B_fB_d interactions.

We study the spectrum properties across the transition by evaluating the Lyapunov coefficient $\gamma(E)$, which is equal to the inverse of the localization length $\ell(E)$, through the asymptotic relation

$$\gamma(E) = [\ell(E)]^{-1} = \lim_{n_s \to \infty} \frac{1}{n_s d} \ln \left| \frac{G_{n_s, n_s}(E)}{G_{1, n_s}(E)} \right|, \quad (5)$$

where $G(E) = (E - H_{B_f})^{-1}$ is the Green's function related to the Hamiltonian H_{B_f} at energy E, and $G_{i,j}(E) = \langle i|G(E)|j\rangle$. The matrix element $G_{1,n_s}(E)$ and G_{n_s,n_s} have been computed by exploiting a renormalization/decimation scheme [23]. The behaviour of the Lyapunov coefficient through the transition is shown

in Fig. 3. The different lines, which correspond to the crosses in Fig. 2, show that the localization length is greater than the system size for points C, D, E. The location of the minima corresponds to the position of the resonance energy $E_{\rm res}$, which moves inside the band for increasing values of |a'|. The nonzero value of γ in the delocalization regime is due to the finite value of n_s in computing Eq. (5) $(n_s=1000$ for the evaluation of γ).

The nature of the states determines the matter-wave transport properties near equilibrium. These can be evaluated by embedding the whole system in a perfect lattice of site energies ϵ_a and hopping energies t_{aa} [22], as previously outlined for the evaluation of the dual-dimer resonance energy. The transmission probability $\mathcal{T} = |\tau|^2$, defined as the squared modulus of the transmission amplitude,

$$\tau = 1 + G_{n_s,1}^0 T_{1,n_s} + G_{1,n_s}^0 T_{n_s,1} e^{-2ik(n_s - 1)a} + G_{n_s,n_s}^0 T_{n_s,n_s} + G_{1,1}^0 T_{1,1},$$
(6)

for different values of a' is shown in the inset of Fig. 3. For $a' = -346 \, a_0$ the resonance fits in the band-edge, and the corresponding transmission peak arises. For $a' = -361 \, a_0$ and $a' = -376 \, a_0$ the peak moves toward the center of the band in agreement with the position of the minimum value of γ . The width of the peak decreases by increasing the system size, as the percentage of the delocalized states scales as $\sqrt{n_s}/n_s$.

Since the condensate energy corresponds to the lowest allowed energy (quasimomentum k=0), the region nearby the resonance could be explored by preparing Bloch states with initial quasimomentum $k \neq 0$ by introducing a constant frequency shift between the two waves generating the lattice [24]. We expect that, in the localization regime, for any $k \in [-\pi/d, \pi/d]$, the whole condensate stays at rest in the reference frame of the moving lattice, while, in the delocalization regime, at $k = k(E_{\rm res})$, the bulk of the condensate stays at rest in the laboratory reference frame.

Both the Lyapunov coefficient and the transmittivity show some small peaks (sinkings). These structures are due to an underlying order present in the procedure illustrated in Fig. 1. In fact, even if our proposition allows the distance between two subsequent impurities to be equal to any integer > 1, still every three sites is definitly without an impurity. The evidence that this underlying order does not affect the DRDM physical effect is shown in Fig. 4. The transmittivity peak for the DRDM pattern proposed in this article (Fig. 1) is in correspondence with the transmittivity peak for a genuine DRDM. Such a disorder pattern could be generated by using a dipolar gas for which repulsive interactions may avoid next-neighboring occupation [25]. However, at the moment of writing, no dipolar gases have yet been cooled down to the degenerate regime in mixtures.

For completeness of our analysis, we compare the two

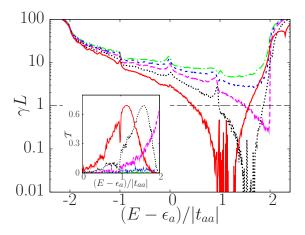


FIG. 3: (Color online) Lyapunov coefficient γ in units of 1/L, $L=n_sa$ being the lattice length, as a function of the energy of bosons B_f . The dot-dashed green line corresponds to point A in Fig. 2, the short-dashed blue line to B, the long-dashed magenta line to C, the dotted black line to D, and the continuous red line to E. The inset shows the corresponding behavior of the transmittivity \mathcal{T} .

DRDM models with a lattice where the position of impurities ϵ_b are uncorrelated [26]. In this case the transmittivity drops (Fig. 4) and becomes vanishing for longer chains. The residual peak is a signature of the presence of a few dual dimers, and it would be washed out in an ordinary disorder model with uncorrelated on-site and hopping energies. It is worth pointing out that the impurity distribution deeply modifies the nature of the states, but not the spectrum itself at this low impurity concentration. Indeed, the density of states (DOS) is essentially the same for the three cases as shown in the inset of Fig. 4. When the percentage of impurities is increased, the underlying periodicity, which is different in the three models, leads to fragmentation of the DOS in three, two, or one band. The DOS, $\mathcal{N}(E)$, has been evaluated by using the Kirkman-Pendry relation $\mathcal{N}(E) = \frac{1}{\pi} \operatorname{Im} \{ [\partial \ln G_{1,n_s}(E)] / (\partial E) \} [27].$

In conclusion, in this work we show that, at fixed correlation function among defects, localization-delocalization can be induced by varying the impurity cross section. In an ultracold boson-boson mixture, where one component plays the role of correlated impurities, the rule being that no next-neighboring impurities are allowed (DRDM), this can be realized by driving the interspecies interaction by means of Feshbach resonances. This is a unique opportunity compared to other physical domains where this class of disorder was previously identified as the possible explanation of the mechanism causing the amazing conducting properties of disordered 1D systems, such as conjugated polymers or biopolymers.

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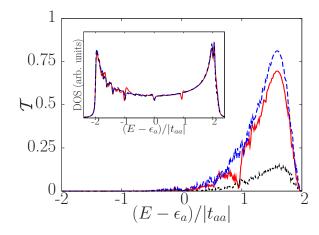


FIG. 4: (Color online) Transmission coefficient \mathcal{T} for $N=1.3\times 10^4$ and $a'=-361\,a_0$, and different disorder patterns: a genuine DRDM lattice (dashed blue line), a DRDM lattice generated with the procedure illustrated in Fig. 1 (continuous red line), and an uncorrelated lattice (dotted black line). The inset shows the corresponding density of states.

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